Novel massless phase of Haldane-gap antiferromagnets in magnetic field

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The behavior of Haldane-gap antiferromagnets in strong magnetic field is not universal. While the low-energy physics of the conventional 1D spin-1 Heisenberg model in its magnetized regime is described by one incommensurate soft mode, other systems with somewhat perturbed coupling constants can possess two characteristic soft modes in a certain range of the field strength. Such a *two*-component Lutinger liquid phase is realised above the massive Haldane-gap phase, and in general above any massive nonmagnetic phase, when the ground state exhibits short range incommensurate fluctuations already in the absence of the field.

Quantum mechanical systems possessing a spectral gap in their ground state are usually very robust: the gap can persist even if relatively large perturbations are added to the Hamiltonian. This is exactly the case for the one-dimensional spin-1 antiferromagnetic chain where the existence of an energy gap, the Haldane gap,[1] is well documented and understood for the Heisenberg model. In the more general SU(2) symmetric bilinear-biquadratic spin-1 model

$$H = \sum_{i=1}^{N-1} \left[\mathbf{S}_i \mathbf{S}_{i+1} + \beta (\mathbf{S}_i \mathbf{S}_{i+1})^2 \right] - h \sum_{i=1}^{N} S_i^z . \qquad (1)$$

in which $\beta = 0$ yields the conventional Heisenberg model, the Haldane gap survives in the whole range $-1 < \beta < 1$, thus there is a large region in the β-space where the biquadratic term has seemingly no effect on the low-energy physics.[2] The Haldane gap disappears in the integrable critical points $\beta = \pm 1$ beyond which new phases appear. For $\beta < -1$ translation invariance is spontaneously broken and dimerization occurs. In the region $\beta > 1$ the bilinear-biquadratic model is believed to remain gapless with soft modes at momenta $k = 0, \pm 2\pi/3$. Since the system is one dimensional no long-range order exists in this phase either: the correlation functions decay algebraically.

The emergence of the Haldane gap in the vicinity of the $\beta = 1$ point, the so called Uimin-Lai-Sutherland (ULS) point,[3] has been investigated recently by Itoi and Kato[4] in the absence of magnetic fields $h = 0$. The ULS model has an SU(3) symmetry which is broken down to SU(2) when β is tuned away from 1. They identified the critical theory of the ULS point with the $k = 1$ SU(3) Wess-Zumino-Witten-Novikov (WZWN) model and concluded that the SU(3) symmetry breaking perturbation, represented by the deviation term with $(\beta - 1)$ in the Hamiltonian, is irrelevant for $\beta > 1$, i.e., the system remains critical there, but it becomes marginally relevant and gives rise to a dynamic mass generation (the Haldane gap) for $\beta < 1$. The transition is of the Berezinskii-Kosterlitz-Thouless (BKT) type, i.e., the gap open exponentially slowly away from the ULS point. These findings are supported by earlier numerical results.[5]

When there is a magnetic field present the SU(2) symmetry of the bilinear-biquadratic model breaks down to U(1). At the ULS point, however, where the symmetry is higher, the quantities N_+, N_0, and N_-, denoting the numbers of $+$, 0, and $-$ spin states in the wave function, with $N_+ + N_0 + N_- = N$ the length of the chain, are independently conserved. Thus the remaining continuous symmetry for $\beta = 1$, $h > 0$ is $U(1) \times U(1)$. For $\beta < 1$ when the strength of the field is higher then the value of the gap, the Haldane gap collapses and the low-energy physics of the magnetized system is governed by gapless excitations. The emerging periodicity is a function of the field strength and in the generic situation incommensurate. Finally, when the field is strong enough all the spins align and the magnetization saturates.

At the ULS point, where the Haldane gap no longer exists, the analysis of the Bethe Ansatz equations showed[6] that the magnetization growth is not smooth.There is a second order phase transition which leads to a cusp in the the magnetization curve $m = m(h)$ at a critical field $h_c \approx 0.941$, $m_c = m(h_c) \approx 0.556$. In the low field regime $h < h_c$, all three probabilities $P_+ = N_+/N$, $P_0 = N_0/N$ and $P_- = N_-/N$ tend to finite values as $N \to \infty$, but for $h > h_c$ the ground state is in a sector with $N_- = 0$, i.e., $P_- = 0$. Thus P_- can be used as an order parameter for the transition. The magnetization behaves continuously at the critical point, but the susceptibility diverges below h_c. The high-field phase (S1 phase), where the low-energy sector is identical to that of the spin-1/2 Heisenberg chain, can be described by a one-component Luttinger liquid, and there is only one characteristic soft mode. The low field phase (S2 phase), on the other hand, is equivalent to a two-component Luttinger liquid, possessing two critical degrees of freedom, and thus *two* incommensurate soft modes. Their positions in the Brillouin zone are functions of the probabilities $P_{+,0,-}$. In the sequel, we label phases by Sn, where $n = 0, 1, 2$ stands for the number of critical, Luttinger liquid components. Note that S0 is a gapped phase.

Early speculations[6,7] that the S2-S1 phase transition of the ULS model may also take place in the Heisenberg chain at $\beta = 0$ was finally refuted by Takahashi and Sakai[8] who found that in the whole range $0 < m < 1$ the low-energy physics is described by a $c = 1$ U(1) conformal field theory (CFT) which is equivalent to the one-component Luttinger liquid, thus only an S1 phase appears. The Luttinger liquid parameters vary smoothly as a function of the magnetization. Naturally arises the question whether the appearence of the Haldane gap in the ground state only allows the S1 behavior seen for the pure Heisenberg model, or there is a certain domain in parameter space where multi-component Luttinger liquids such as an S2 phase can occur above the S0 Haldane phase. To clarify this question is the principal aim of this Letter.

The first indication that the Haldane gap of the bilinear-biquadratic model may collapse into an S2 phase comes from the numerical observation that at $h = 0$ the VBS point $\beta_{\mathrm{VBS}} = 1/3$, where the ground state can be constructed exactly using nearest-neighbor valence bonds, is in fact a disorder point, beyond which short range fluctuations in the ground state become incommensurate.[9] However, due to the finite correlation length, the peak at π in the static structure factor only splits somewhat later at the so called Lifshitz point $\beta_{\mathrm{Lifs}} \approx 0.438$.[9] One can define a third special point β_{Disp}, which is *a priori* distinct from (but close to) the above two, where the emerging incommensurability make the position of the minimum gap in the energy-momentum dispersion relation move away from π. In the range $\beta_{\mathrm{Disp}} < \beta < 1$ the momentum p_{H} associated with this gap minimum rapidly shifts from the antiferromagnetic value π to the ULS value $2\pi/3$. When the magnetic field reaches the value of the gap at p_{H}, and the system starts to become magnetized, there are obviously two characteristic momenta in the system: one is $2\pi m$, as suggested by the generalization of the Lieb-Schultz-Mattis theorem,[11] and the other is the finite difference of the two split gap minima $2p_{\mathrm{H}}$. Of course, any linear combinations of these two may also show up in the correlation functions, which will be dominated by the most slowly decaying terms, or on shorter distances, by the ones having the largest amplitude.

A more quantitative analysis is possible on the basis of the Bethe Ansatz (BA) solution of the ULS model, when the deviation term proportional to $(1-\beta)$ in the Hamiltonian is treated as a perturbation. The ULS model is solvable by the two-component nested BA method.[3] This associates the $+$ spin states with an inert background in which particles with two possible internal states, spin 0 and $-$, move. Two sets of spectral parameters are introduced, one for the particles (component-1) and one for their internal state (component-2). Their actual values can be calculated by solving a set of coupled algebraic (or in the $N \to \infty$ limit integral) equations. The BA technique also allows one to obtain the finite size corrections $\mathcal{O}(1/N)$ to the low-energy excitations near the thermodynamic limit. In the S2 phase of the ULS model the energy spectrum has the following structure:[10]

$$\delta E = E_{\mathbf{a}} - E_g = \frac{2\pi}{N}\left[v_1(\Delta_1^+ + \Delta_1^-) + v_2(\Delta_2^+ + \Delta_2^-)\right] \quad (2)$$

with

$$\Delta_1^\pm = \frac{1}{2}\left[Z_{11}d_1 + Z_{21}d_2 \pm \frac{Z_{22}l_1 - Z_{12}l_2}{2\det Z}\right]^2 + n_1^\pm$$
$$\Delta_2^\pm = \frac{1}{2}\left[Z_{12}d_1 + Z_{22}d_2 \mp \frac{Z_{21}l_1 - Z_{11}l_2}{2\det Z}\right]^2 + n_2^\pm \quad (3)$$

where E_g is the energy of the ground state, the index $\mathbf{a} \equiv \{d_1, d_2; l_1, l_2; n_1^+, n_1^-, n_2^+, n_2^-\}$ is a shorthand for eight integer (half-integer) quantum numbers specifying the eigenstate, and the matrix $Z_{\alpha\beta}$, $\alpha, \beta = 1, 2$ is the "dressed charge matrix" responsible for the interaction of the two BA components. The relative momentum of the state $\mathbf{a}$ reads

$$\delta P = P_{\mathbf{a}} - P_g = Q + \frac{2\pi}{N}(\Delta_1^+ - \Delta_1^- + \Delta_2^+ - \Delta_2^-) \quad (4)$$

where $Q = Q_{\mathbf{a}}$ is an $\mathcal{O}(1)$ term

$$Q = 2\pi(1-P_+)d_1 + 2\pi P_- d_2 + \pi l_1. \quad (5)$$

The physical interpretation of the quantum numbers is as follows: l_α (d_α) represents the number of particles added to (transferred from the left Fermi point to the right in) component α. $n_\alpha^\pm$ is the number of small momentum particle-hole pairs created in component α around the left ($-$) and the right ($+$) Fermi points. While l_α and $n_\alpha^\pm \geq 0$ are always integers, d_α is integer or half integer with $d_{1,2} \equiv l_{2,1}/2 \pmod 1$.[13] This structure is analogous to the one found in the 1D Hubbard model where the two components are called "charge" and "spin", resp. In the present case $l_1 = \delta N_0 + \delta N_-$, $l_2 = \delta N_-$ for which there are selection rules when a given type of correlation functions is considered.

The low-energy excitations of the ULS model in its S2 phase can be interpreted by assuming that they arise from the direct sum of two $c = 1$ conformal field theories (CFT) each having a different sound velocity v_1 and v_2, resp.[10] As is indicated by Eq. (3) local physical operators necessarily couple to both CFTs. Conformal invariance then requires that the 2-point functions behave as[10]

$$\langle\phi(x,t)\phi(0,0)\rangle = A_\phi e^{-iQx}\prod_{\alpha,\pm}(x \mp iv_\alpha t)^{-2\Delta_\alpha^\pm} \quad (6)$$

showing the analog of "spin-charge separation" for the present spin-1 situation. Let us consider the operator content of the theory: each operator $\phi_{\mathbf{a}}$ (primary or secondary) is labeled by the eight quantum numbers $\mathbf{a}$, and has the anomalous dimension $x_{\mathbf{a}} = \Delta_1^+ + \Delta_1^- + \Delta_2^+ + \Delta_2^-$ and conformal spin $s_{\mathbf{a}} = \Delta_1^+ - \Delta_1^- + \Delta_2^+ - \Delta_2^- = d_1 l_1 + d_2 l_2 + n_1^+ - n_1^- + n_2^+ - n_2^-$. Note that the total momentum associated to these operators is δP in Eq. (4), involving the Q term as well. There are four marginal operators $\mathcal{M}_{1,2,3,4}$ which can be formed using only the $n_{1,2}^\pm$

quantum numbers and setting $l_\alpha, d_\alpha = 0$. Their dimension, spin and total momentum ($x = 2,\ s = 0,\ \delta P = 0$) do not depend on the $Z_{\alpha\beta}$ matrix. The presence of these operators causes the existence of an extended critical domain in the parameter space. The other relevant or marginal operators are all primary, i.e., $n_\alpha^\pm = 0$ and all depend on the $Z_{\alpha\beta}$ matrix. This latter can be calculated numerically for the ULS model by solving a set of coupled integral equations. The results[12] are shown in Fig. 1(a). When $h = 0$, $Z_{11} = Z_{22} = \sqrt{1/3 + 1/2\sqrt{3}}$, $Z_{12} = Z_{21} = \sqrt{1/3 - 1/2\sqrt{3}}$, and there is an additional marginal operator $\phi_{1/2,1/2;1,-1}$ (and its equivalents under SU(3) and parity transformations, e.g., $\phi_{1,1}$) as can be checked using Eq. (3). (From now on in the index $\mathbf{a}$ we omit l_α and/or $n_\alpha^\pm$ when they are zero.) The operator $\phi_{1/2,1/2;1,-1}$ has anomalous dimension $x = 2$ and total momentum $\delta P = 0$ when $h = 0$. This is the principal operator responsible for the SU(3)→SU(2) symmetry breaking processes $00 \longleftrightarrow +-, -+$. As was shown in Ref.[4] the interplay of $\phi_{1/2,1/2;1,-1}$ and the $\mathcal{M}$ operators (which constitute the SU(3) current interaction in the WZWN theory) gives rise to the Haldane gap for $\beta < 1$ but maintains criticality for $\beta > 1$.

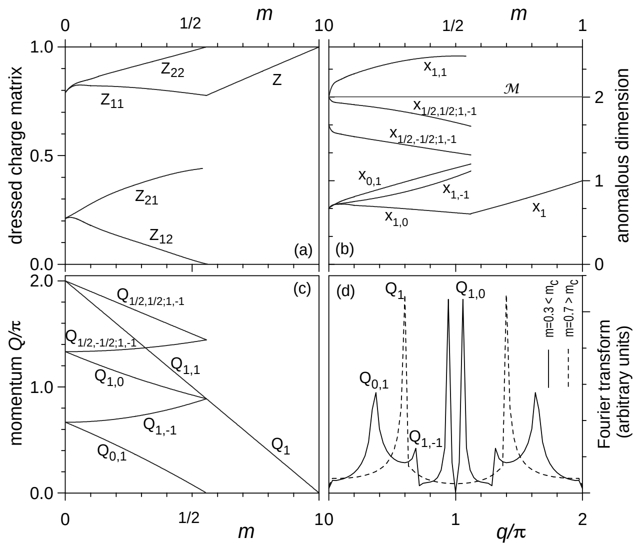

FIG. 1. Bethe Ansatz results for the ULS model vs the magnetization m. (a) The dressed charge matrix, (b) anomalous dimension and (c) momentum Q of some selected operators. Some other operators marginal at $h = 0$ are not shown. (d) DMRG results for the Fourier transform of the one-point function $\langle S_n^z \rangle$. The peak at the Lieb-Schultz-Mattis value $q = 2\pi m, 2\pi(1 - m)$ only develops for $m > m_c$.

When $0 < h < h_c$ the anomalous dimensions and momenta of the operators present in the ULS model vary as shown in Fig. 1(b). Since the perturbation part of the Hamiltonian, represented by the deviation $(1 - \beta)$ term, transforms under translations with momentum zero, in its decomposition into the operators present in the ULS model at $h > 0$ only operators with $\delta P = 0$ can appear. This is a serious limitation, since as shown in Fig. 1(c), the two characteristic momenta $Q_{1,0} = 2\pi(1 - P_+)$ and $Q_{0,1} = 2\pi P_-$, associated to the large momentum transfer processes of the two components in Eq. (5), become generically incommensurate. $\phi_{1/2,1/2;1,-1}$ has no longer $\delta P = 0$ so it does not contribute. It is in fact an Umklapp operator which appears in the low-energy description only at $h = 0$. What contribute are the operators $\phi_{d_1,d_2;1,-1;n_1^\pm;n_2^\pm}$ with d_1, d_2 half-integer, and $n_\alpha^\pm > 0$ chosen in a way to reinstall $\delta P = 0$. However, due to the appearance of the necessary small momentum particle-hole excitations such operators are highly irrelevant. The marginal operators $\mathcal{M}$ are not able alone to drive the two Luttinger liquid components away from criticality, although they make the universality class change continuously. We conclude that when $0 < m < m_c$ the bilinear-biquadratic model must remain in its S2 phase in an extended domain on *both* sides of the ULS line $\beta = 1$.

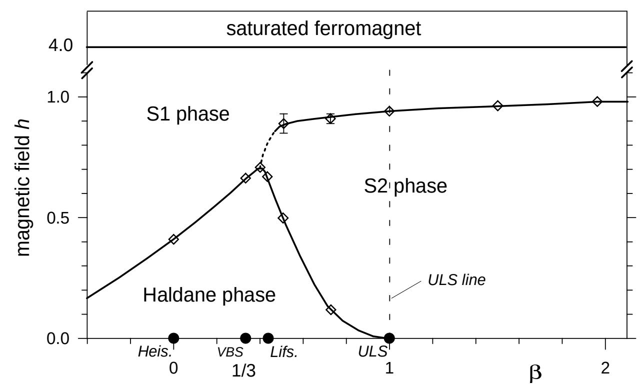

FIG. 2. Phase diagram of the bilinear-biquadratic spin-1 chain in a magnetic field. The one- and two-component Luttinger liquid phases are denoted by S1 and S2, resp. The S1–S2 phase boundary is determined by the DMRG ($\diamond$ points). The dotted line indicates some uncertainties near the disorder points.

When the magnetic field reaches the critical value h_c in the ULS model the sound velocity $v_2 \to 0$, and the corresponding critical degree of freedom becomes massive. The emerging S1 phase can be described by a single $c = 1$ CFT, and the universality class is determined by a scalar dressed charge Z. Once again we do not expect any drastical changes in the low-energy physics as β is perturbed away from 1. The predicted phase diagram is shown in Fig. 2.

In order to find the exact phase boundaries we carried out a detailed numerical analysis using the DMRG technique. Unfortunately the DMRG does not work in momentum space thus a direct search for tracking soft modes by calculating energy gaps is not feasible. Instead, we calculated the decay of the one-point function $\langle S_j^z \rangle$ from the edge of an open chain for different values of β and magnetization $m = S^z_{\rm tot}/N$. The one-point function contain the same information as the equal time two-point correlation function in Eq. (6) (note that the

exponent of the one-point function is half of that of the two-point function), and the appearing soft modes can be identified in the Fourier transforms or by making a suitable multi-parameter fit in real space.[12]

Once again exact results can be obtained for the ULS model. Considering $\langle S_j^z \rangle$ in the S2 phase only operators with $\delta S^z_{\rm tot} = 0$, i.e., $l_1 = l_2 = 0$ and $l_1 = -l_2 = \pm 1$ can contribute. The most relevant operators are $\phi_{1,0}$, $\phi_{0,1}$, $\phi_{1,-1}$, $\phi_{1/2,1/2;1,-1}$, and $\phi_{1/2,-1/2;1,-1}$ (and their equivalents under symmetries). The associated momenta Q (position of the peak in the structure factor) and the occurring critical exponents can be read off from Fig. 1(b) and (c). The example presented in Fig. 1(d) illustrates that in the S2 phase of the ULS model only the first three with $l_1 = l_2 = 0$ have nonvanishing amplitude as dictated by the higher symmetry. However, $\phi_{1/2,\pm 1/2;1,-1}$ contributes when $\beta \neq 1$. It is remarkable that in the S2 phase the operator $\phi_{1,1}$, which has an anomalous dimension over 2 and momentum $Q_{1,1} = 2\pi(1-m)$, does not contribute to the correlation function. In the high-field S1 phase, however, the only peak discernible in the structure factor, as shown in Fig. 1(d), is the one with $Q_1 = 2\pi(1-m)$, in agreement with the Lieb-Schultz-Mattis theorem.[11] The presence or absence of a peak in the structure factor at $k = \pm 2\pi m$ can thus be used efficiently to distinguish between the two phases and locate the phase boundary. Alternatively, one can monitor the amplitude of the peak at $Q_{0,1}$ which tends to zero on the transition line where the multi-peak structure collapses into a single-peak one. The phase diagram, as determined by the DMRG calculation, is shown in Fig. 2. Details of the numerical investigation will be published elsewhere.[12]

Our analysis is valid in the strict sense close to the ULS line only. Here the S2–S1 phase transition is clearly associated to the depletion of one of the two "bands" as suggested by the BA. Note that in Fig. 2 the phase boundary does not change very much until about $\beta \sim 0.5$ where it seems to decline rather rapidly. *A priori* we cannot exclude the possibility that some operators become relevant here and open a gap in one of the critical components. This question needs further clarification.

In the bilinear-biquadratic model in Eq. (1) the S2 phase terminates near $\beta \approx 0.4$. This is still far in the parameter space from the currently known spin-1 Haldane gap materials for which the biquadratic term is small, and the pure Heisenberg model, although with some anisotropies, is a good description. For these systems only S1 type massless phases (and eventually, for some special values of m, additional S0 type phases, i.e., magnetization plateaus[11,14]) are expected to appear. However, even here, due to the closeness of the S2 phase somewhat further in the phase diagram, massive but relatively low energy excitations are predicted to show up in the weakly magnetized regime. They are expected to contribute in experiments probing higher lying excitations such as in inelastic neutron scattering, or in situations when short distance physics is important as, e.g., in nonmagnetically doped materials. Although there is no sharp phase transition in this case, the low-field and high-field regimes may look rather different, separated by a more or less narrow crossover region as observed, e.g., in Ref. 7.

In general, a two-component Luttinger liquid phase (S2), and then an eventual phase transition S2→S1 during the magnetization process, is expected to occur whenever the ground state develops incommensurate fluctuations already at $h = 0$. It must not necessarily be above a Haldane gap; the spin-1/2 zig-zag ladder, for example, which is expected to describe adequately the quasi-1D antiferromagnet Cs_2CuCl_4, where the gap is due to dimerization and fluctuations are also predicted to be incommensurate already without a magnetic field,[15] is another possible candidate.

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